

Thursday, April 4, 2013

QM Motion in a periodic potential (continued)

Bloch Theorem:

The Hamiltonian eigenstates for a particle in a periodic potential are plane-wave like, and have the form:

$$\langle x | \phi \rangle = \Psi_k(x) = e^{ikx} \underbrace{u_k(x)}_{\substack{\text{determined} \\ \text{by } V(x)}}, \text{ where } u_k(x) \text{ is a periodic function of period } \underline{a}$$

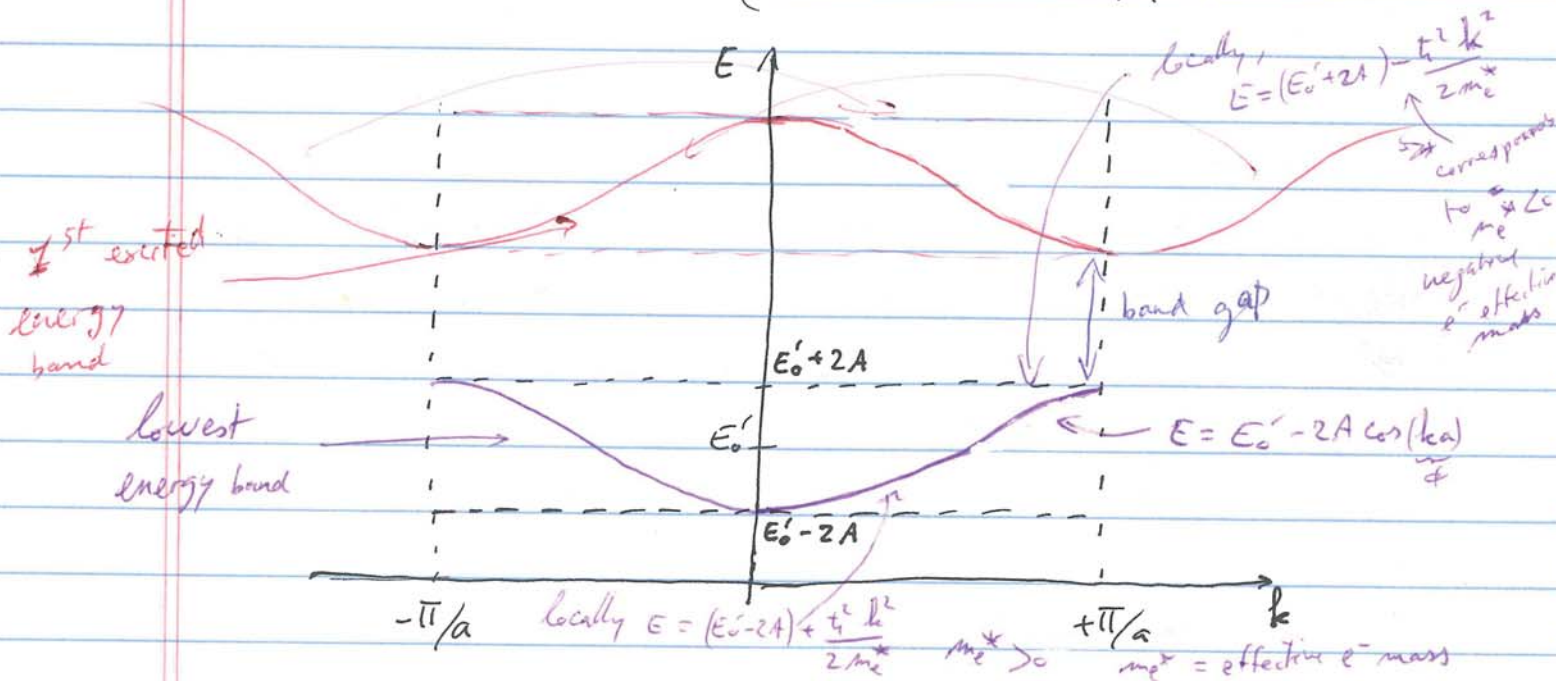
$$u_k(x+a) = u_k(x)$$

$\Psi_k(x)$ is an eigenstate of H and $T(a)$.

Tight binding model

We found that for our model $ka = \phi$

$$H | \Psi_k \rangle = H | \phi \rangle = (E_0' - 2A \cos \phi) | \phi \rangle = (E_0' - 2A \cos(ka)) | \Psi_k \rangle$$

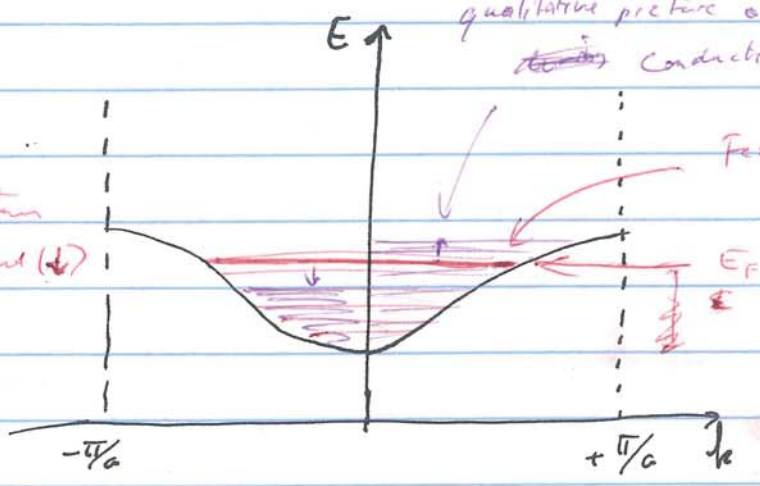


Metals have ~~unfilled~~ a partially filled ~~valence~~ valence energy band.

Pauli Principle

$2e^-$ per momentum state (\uparrow) and (\downarrow)

qualitative picture of conduction
~~conduction~~ conduction = unbalanced distribution of momenta

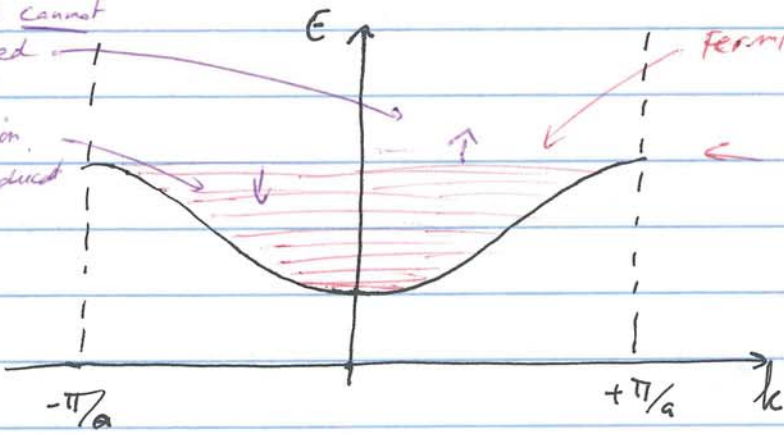


Insulators have a completely full valence energy band

e^- 's cannot be redistributed to create an unbalanced distribution

population cannot be increased here
 population could be reduced here

Fermi Surface

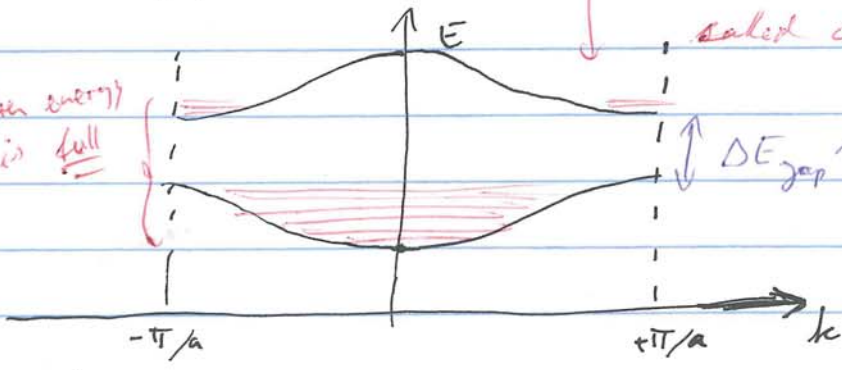


Semiconductors have a completely full valence energy band that thermally populates the first excited band due to the ~~small~~ band gap ΔE being ~~on~~ the order of the thermal energy

neither energy band is full

valence conduction band

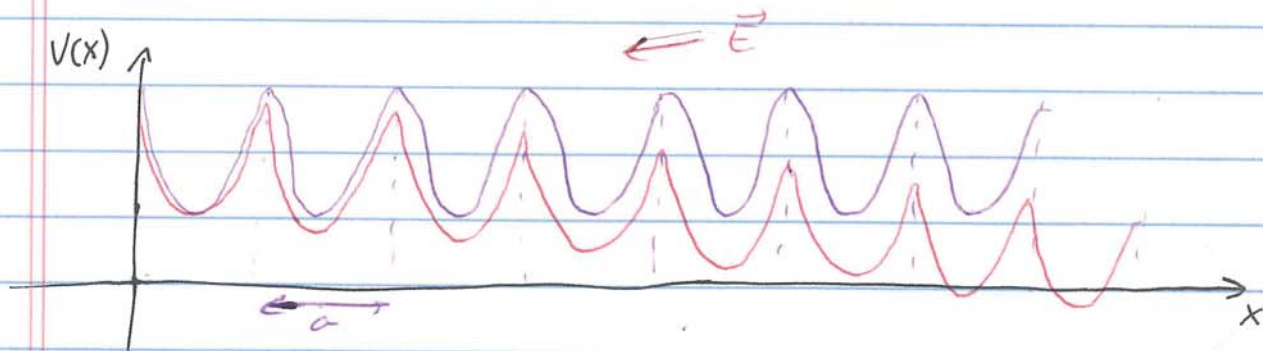
$\Delta E_{gap} \sim kT$



Block oscillations

Consider a periodic potential for an e^- subject to an E -field

$$H = \frac{p^2}{2m_0} + V_{\text{periodic lattice}}(x) - q_e E x$$



This is a model for conduction of e^- 's in a crystal lattice.

- Classically, if we permit e^- 's to tunnel, then we expect e^- motion to the right ($+x$).
- Quantum Mechanically, we find that the reflection of e^- 's off the lattice barriers as they move right leads to a constructive interference phenomenon, where the ~~the~~ e^- 's oscillate back and forth (at frequency $\omega_{\text{Bloch}} = \frac{a q_e |E|}{\hbar}$) without making progress to the right.

~~the~~

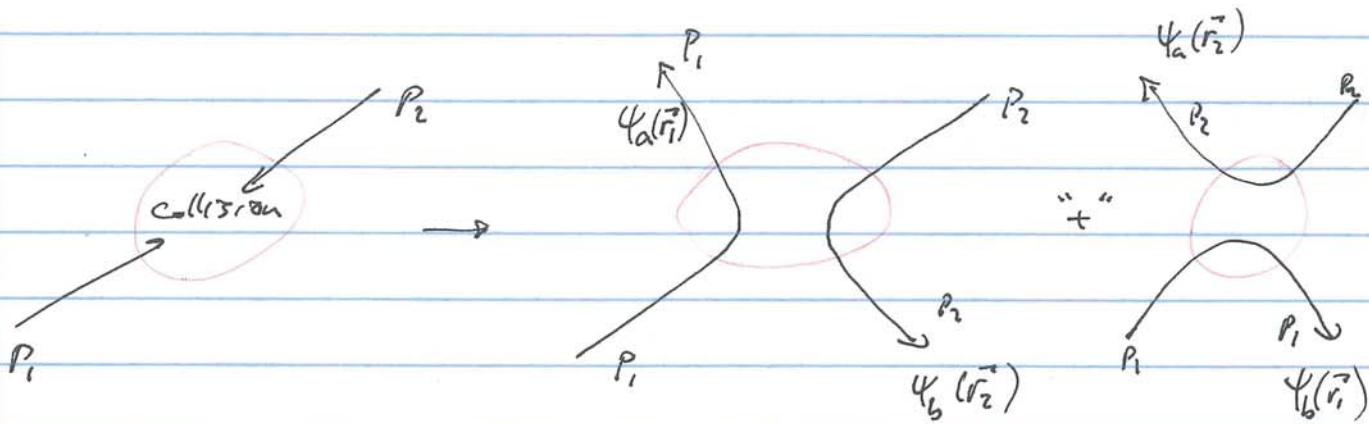
This conduction paradox is resolved because in real metals the e^- 's scatter off each other, phonons, and impurities. These scattering processes dephase the reflections enough to wash out the interference effects.

→ Bloch oscillations are very difficult to observe with e^- 's in crystal, but easy with ~~with~~ ~~the~~ ultracold atoms in an optical lattice.

Identical particles: Quantum Statistics

Two identical particles

Consider a collision between 2 identical particles



The final two-particle state is

$$\psi_f(\vec{r}_1, \vec{r}_2) = \psi_a(\vec{r}_1)\psi_b(\vec{r}_2) + e^{i\phi} \psi_b(\vec{r}_1)\psi_a(\vec{r}_2)$$

If you exchange particles 1 & 2, then

$$1 \leftrightarrow 2 : \psi_f(\vec{r}_2, \vec{r}_1) = \psi_a(\vec{r}_2)\psi_b(\vec{r}_1) + e^{i\phi} \psi_b(\vec{r}_2)\psi_a(\vec{r}_1)$$

define the permutation operator P: *interchanging two identical particles should not really change the wavefunction*

$$P \psi(\vec{r}_1, \vec{r}_2) = \psi(\vec{r}_2, \vec{r}_1) \stackrel{?}{=} e^{i\delta} \psi(\vec{r}_1, \vec{r}_2)$$

However, we require $P^2 \psi(\vec{r}_1, \vec{r}_2) = \psi(\vec{r}_1, \vec{r}_2) \stackrel{?}{=} e^{2i\delta} \psi(\vec{r}_1, \vec{r}_2)$

$$\Rightarrow e^{i2\delta} = 1 \Rightarrow \delta = 0 \text{ or } \pi$$

\Rightarrow eigenvalues of P are ± 1
 \rightarrow symmetric
 \rightarrow anti-symmetric

Bosons Permutation Symmetry

Identical Bosons are particles whose wavefunction is symmetric under exchange of any two particles.

2 particles: $\psi(\vec{r}_1, \vec{r}_2) = +\psi(\vec{r}_2, \vec{r}_1) = \frac{1}{\sqrt{2}} \left[\psi_a(\vec{r}_1)\psi_b(\vec{r}_2) + \psi_b(\vec{r}_1)\psi_a(\vec{r}_2) \right]$
 $P\psi(\vec{r}_1, \vec{r}_2) = +\psi(\vec{r}_2, \vec{r}_1)$

N particles: $\psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_i, \dots, \vec{r}_j, \dots, \vec{r}_N)$
 $= +\psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_j, \dots, \vec{r}_i, \dots, \vec{r}_N)$

special case: if only one state is available, the $\psi(\vec{r}_1, \dots, \vec{r}_N) = \psi_a(\vec{r}_1) \dots \psi_a(\vec{r}_N)$
 (i.e. BEC)

Identical Fermions are particles whose wavefunction is anti-symmetric under exchange of any two particles.

2 particles: $\psi(\vec{r}_1, \vec{r}_2) = -\psi(\vec{r}_2, \vec{r}_1) = \frac{1}{\sqrt{2}} \left[\psi_a(\vec{r}_1)\psi_b(\vec{r}_2) - \psi_b(\vec{r}_1)\psi_a(\vec{r}_2) \right]$
 $P\psi(\vec{r}_1, \vec{r}_2) = -\psi(\vec{r}_2, \vec{r}_1)$

N particles: $\psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_i, \dots, \vec{r}_j, \dots, \vec{r}_N)$
 $= -\psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_j, \dots, \vec{r}_i, \dots, \vec{r}_N)$

~~special case~~ Note: - you cannot construct an anti-symmetric wavefunction with only a single state

- Each identical fermion must be in a different state, otherwise anti-symmetry is not possible.

↳ Pauli exclusion principle

↳ responsible for ~~most of chemistry~~ ^{chemical differences} between elements